Ethanone, 1-(2,4-dihydroxyphenyl)-89-84-9 | DTXSID4058998

89-84-9 DTXSID4058998				

Model Performance

Model	Data

Weighted KNN model

5-fold CV (5-fold CV (75%)		Training (75%)		Test (25%)	
Q2	RMSE	R2	RMSE	R2	RMSE	
0.87	0.81	0.87	0.82	0.86	0.86	

Model Results

Predicted value: 5.30e-01 mol/L

Global applicability domain: Inside

Local applicability domain index: 5.13e-01

Confidence level: 5.79e-01

Nearest Neighbors from the Training Set

Image not found

2,2-Bis(bromomethyl)-1,3-

propanediol

Measured: 1.45e-01 Predicted: 2.34e-01

Image not found

Tribromoacetic acid Measured: 6.74e-01 Predicted: 5.34e-01

Image not found

Dibromoacetic acid Measured: 9.69 Predicted: 4.01